United States Environmental Protection Agency

CMAQv5.3.2 ozone simulations over the Northern Hemisphere: model performance and sensitivity to model configuration

Christian Hogrefe[1], Robert Gilliam[1], Rohit Mathur[1], Barron Henderson[1], Golam Sarwar[1], K. Wyat Appel[1], George Pouliot[1], Jeff Willison[1], Rebecca Miller[2], Jeff Vukovich[1], Alison Eyth[1], Kevin Talgo[3], Chris Allen[3], and Kristen Foley[1]

[1]U.S. Environmental Protection Agency, Research Triangle Park, NC, USA
[2]ORAU NSSC, on assignment to U.S. Environmental Protection Agency, Research Triangle Park, NC, USA
[3]GDIT, Research Triangle Park, NC, USA

20th Annual CMAS Conference
November 1 - 5, 2021

Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA.

Scope and Objectives of 2002 – 2017 Hemispheric CMAQ (H-CMAQ) Simulations

- Performed as part of the **E**PA's Air **QUA**lity **T**im**E** **S**eries (EQUATES) project
- Characterize large-scale atmospheric composition to provide boundary conditions for the 12km EQUATES simulations
- Evaluate the modeling system's ability to capture trends and variability in large-scale atmospheric composition
- Use modeling platform to quantify the effects of alternate emission inputs and/or process representations
- Make data available to the community for creating boundary conditions for domains within the Northern Hemisphere

Model Configuration

- **Domain:** Northern Hemisphere at 108 km grid spacing and 44 vertical layers up to 50 mb
- **WRF:** v4.1.1, KF convective scheme with trigger 2, PX land surface model, ACM2 PBL scheme, MODIS land use, Morrison microphysics, RRTMg radiation, no lightning assimilation
- **CMAQ:** v5.3.2 (modified as detailed on slides 4-5), cb6r3m_ae7_kmtbr, STAGE dry deposition (no bi-directional NH_3 flux), potential vorticity (PV) scaling for stratospheric ozone, windblown dust, time-invariant profile-based boundary conditions

- **Emissions (also see Foley et al. 2020 CMAS presentation):**
  - Anthropogenic:
    - U.S.: EQUATES 12 km emissions patched into the 108 km domain
    - Non-US: 2010 HTAP with year-specific scaling from CEDS and Tsinghua University
  - Fires: BlueSky Pipeline (U.S.) and FINN (non-U.S.)
  - Lightning: GEIA climatology
  - Biogenic VOC: CAMSv2.1 (based on MEGAN2)
  - Soil NO: CAMSv2.1 (Yienger and Levy, 1995 with updates based on recent literature)

Observations Used for Model Evaluation

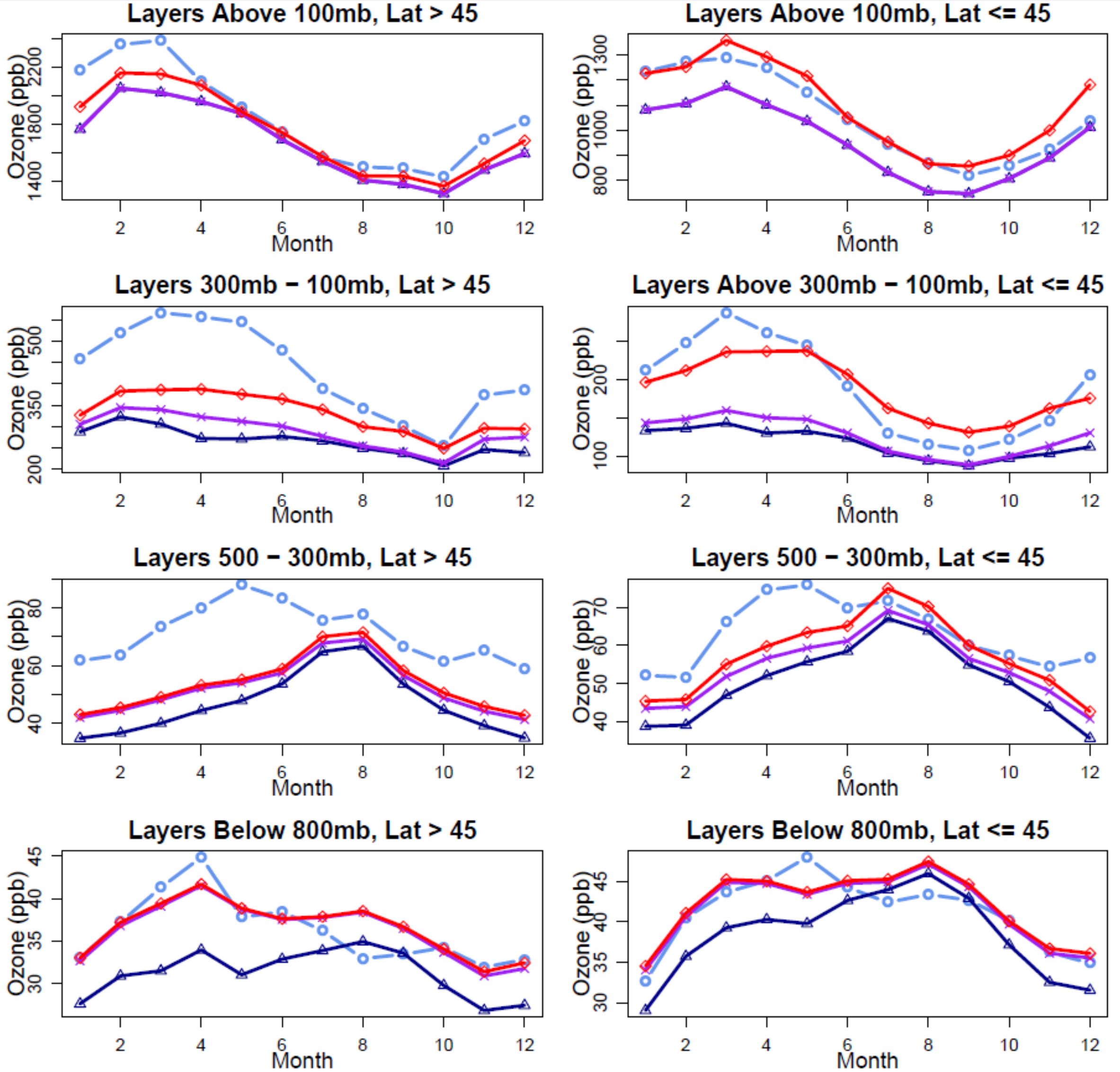
- Surface observations:
  - AQS, CASTNET, NAPS
  - EMEP
  - Tropospheric Ozone Assessment Report (TOAR) database
- Ozonesondes:
  - WOUDC data archive
  - NOAA ESRL data archive
- Satellite:
  - OMI tropospheric ozone column (PROFOZ product) level 2 data processed with cmaqsatproc (https://github.com/barronh/cmaqsatproc)
    - Liu et al., 2010, Atmos. Chem. Phys., 10, doi:10.5194/acp-10-2521-2010
    - Kim et al., 2013, Atmos. Chem. Phys., 13, doi:10.5194/acp-13-9321- 2013

Modifications to CMAQv5.3.2

- Initial simulations for 2010 indicated a substantial underprediction of upper tropospheric O_3 relative to both ozonesondes observations and earlier studies, particularly in winter and spring
- Tested and implemented changes to
  - Detailed halogen chemistry:
    - Had been updated in CMAQv5.3 and increased O_3 loss compared to earlier versions
    - New updates for the EQUATES H-CMAQ simulations consider only sea salt instead of total aerosol surface area for heterogeneous reactions and turn off uncertain bromine cloud chemistry
    - These and other updates are expected to be released in CMAQv6
  - Estimation of stratospheric O_3 based on PV
    - Current parameterization had been developed using 1990 – 2010 WRFv3.4 PV and observed ozonesonde data
    - Confirmed validity of current parameterization with 2002 – 2017 WRFv4.1.1 PV and observed ozonesonde data, but restricted its application to the top model layer only

Effect of Modifications to CMAQv5.3.2

2010 Monthly Mean O_3, All Ozonesonde Sites, 4 Layer Ranges and 2 Latitude Ranges



Observations
CMAQv5.3.2
Revised halogen chemistry, existing O_3-PV scaling
Revised halogen chemistry, O_3-PV scaling top layer only

Revised halogen chemistry effects most pronounced in lower and mid troposphere

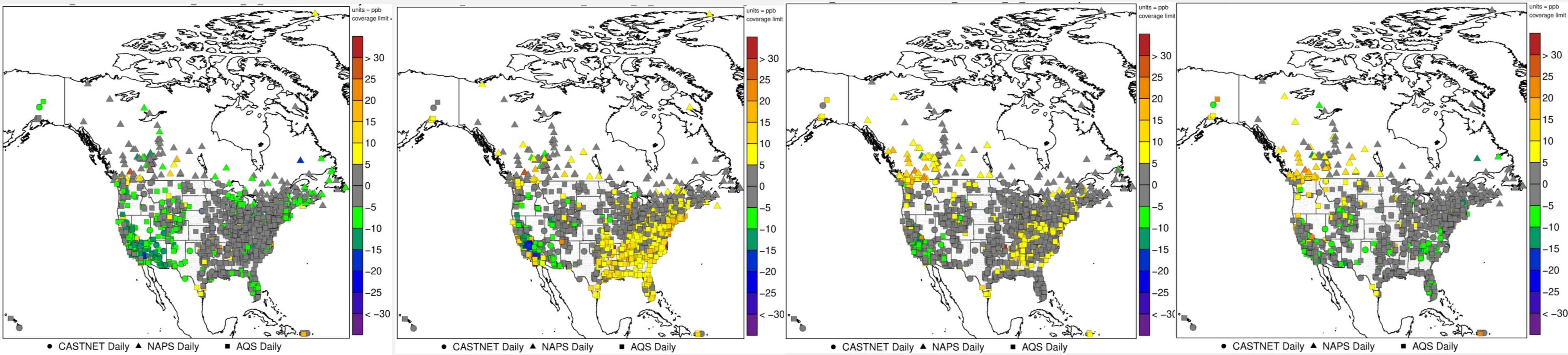
Revised O_3-PV scaling effects most pronounced in upper troposphere

The modifications improve model performance for tropospheric O_3, though springtime underpredictions remain

Implemented these modifications in the 2002 – 2017 simulations

Seasonal Surface MDA8 O_3 Bias, 2002 - 2017

Spring Summer Fall Winter



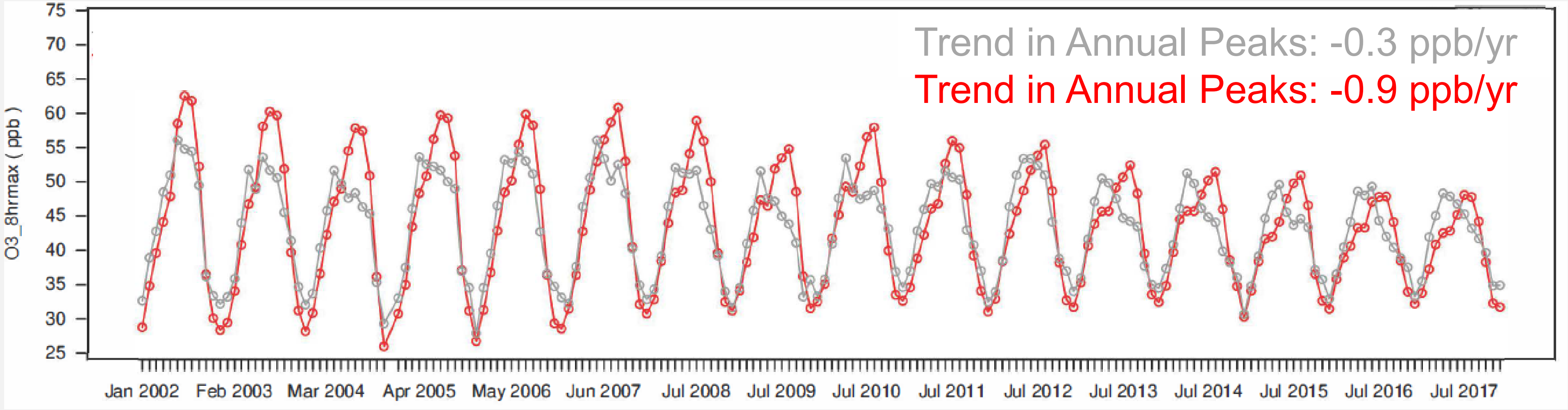
Widespread negative springtime bias in the Western U.S.

Pronounced positive summertime bias in the Southeastern U.S., persisting into the fall

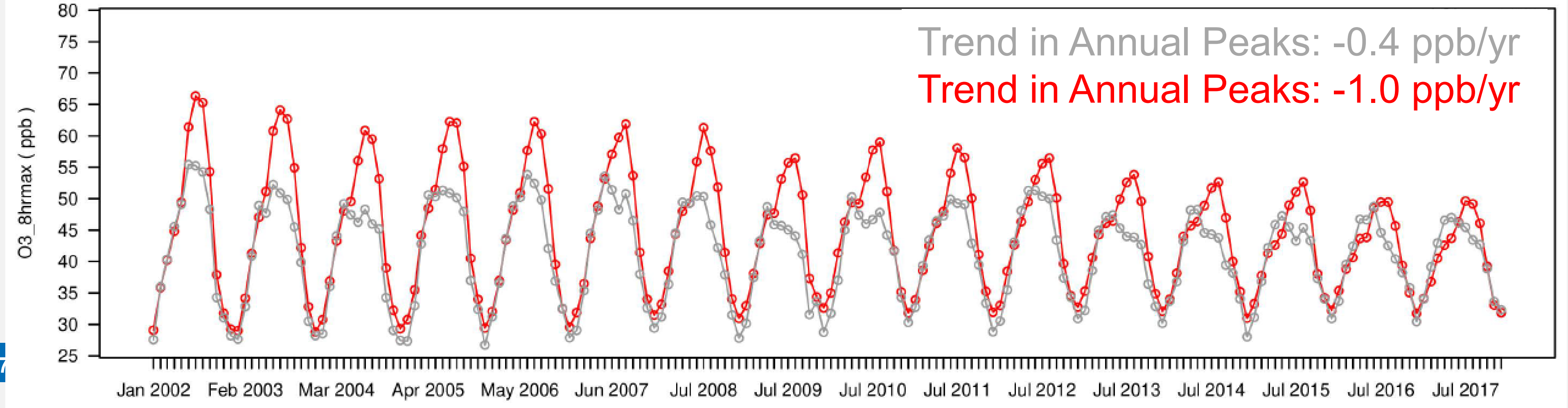
Positive biases in the Pacific Northwest during fall and winter

Monthly Mean Surface MDA8 O_3, CASTNET and AQS

CASTNET



AQS



Observations

H-CMAQ

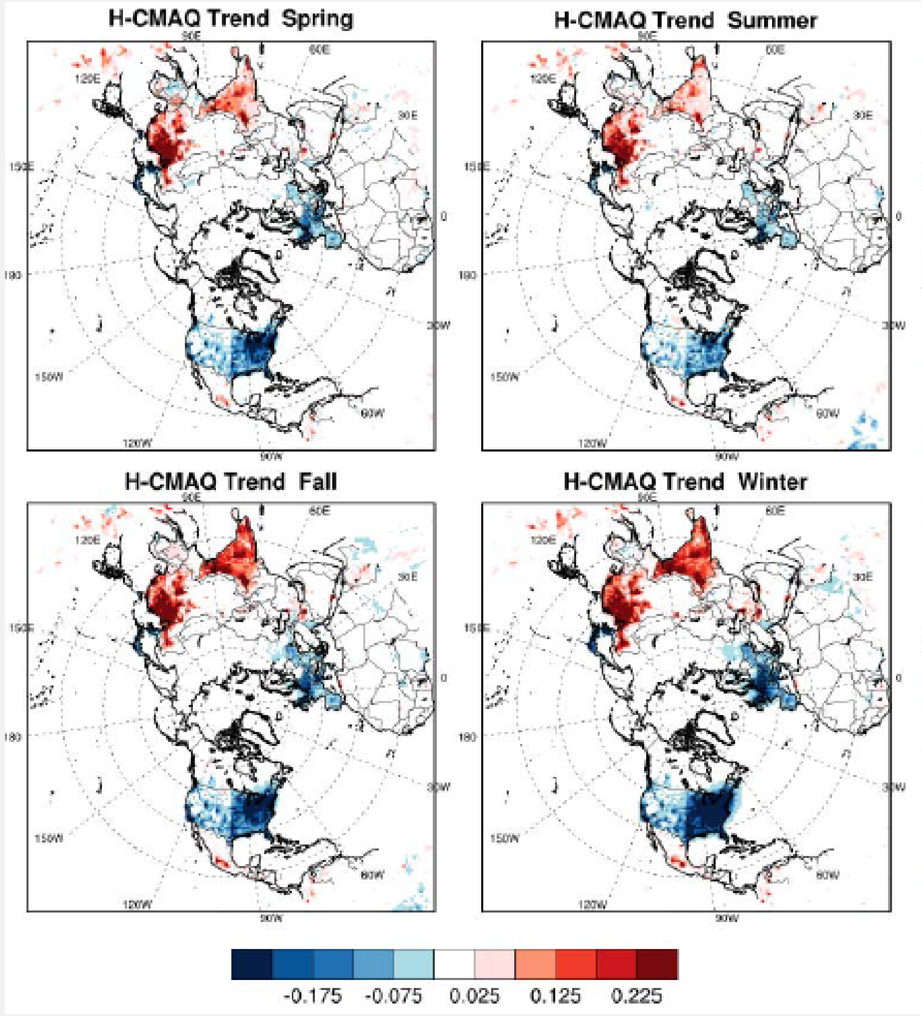
Persistent summertime O_3 overpredictions and tendency to underestimate springtime O_3 (more pronounced at CASTNET sites)

Model shows a stronger downward trend in summertime O_3 than observations

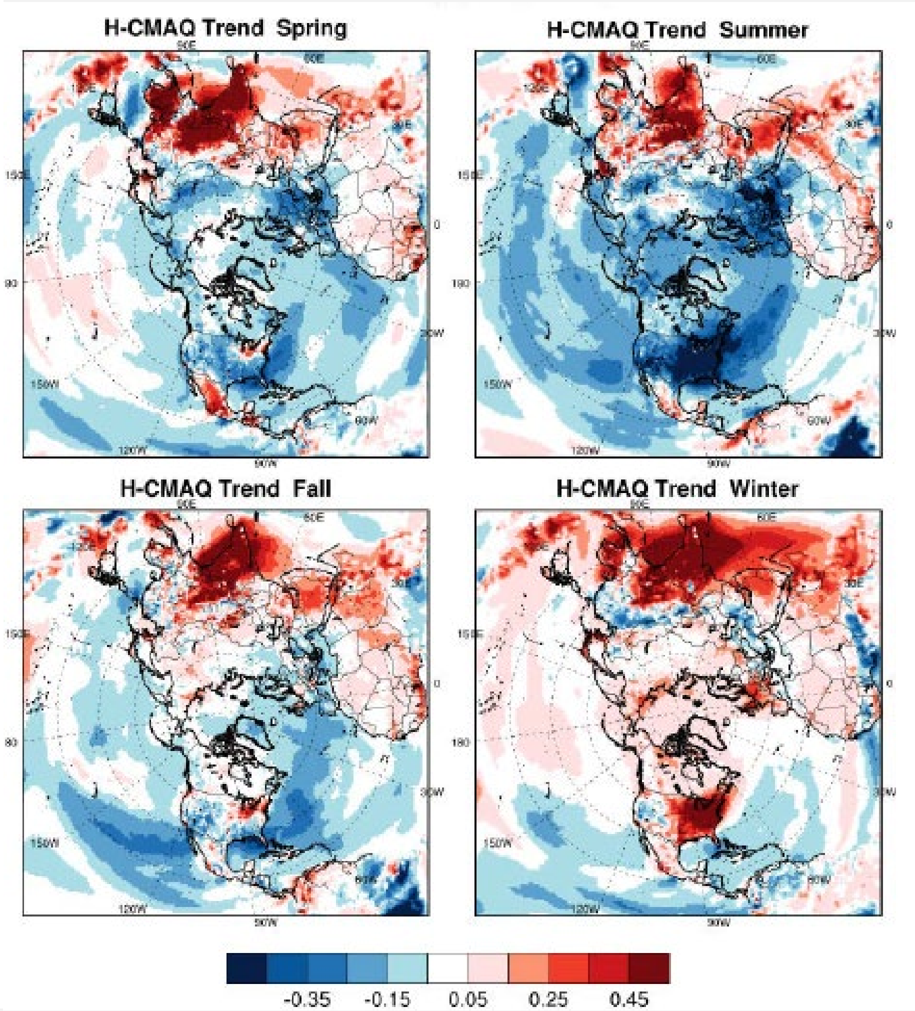
EPA United States Environmental Protection Agency

2002 – 2017 Modeled Surface NO_2 and O_3 Trends

NO_2 Trends (ppb/year)



O_3 Trends (ppb/year)



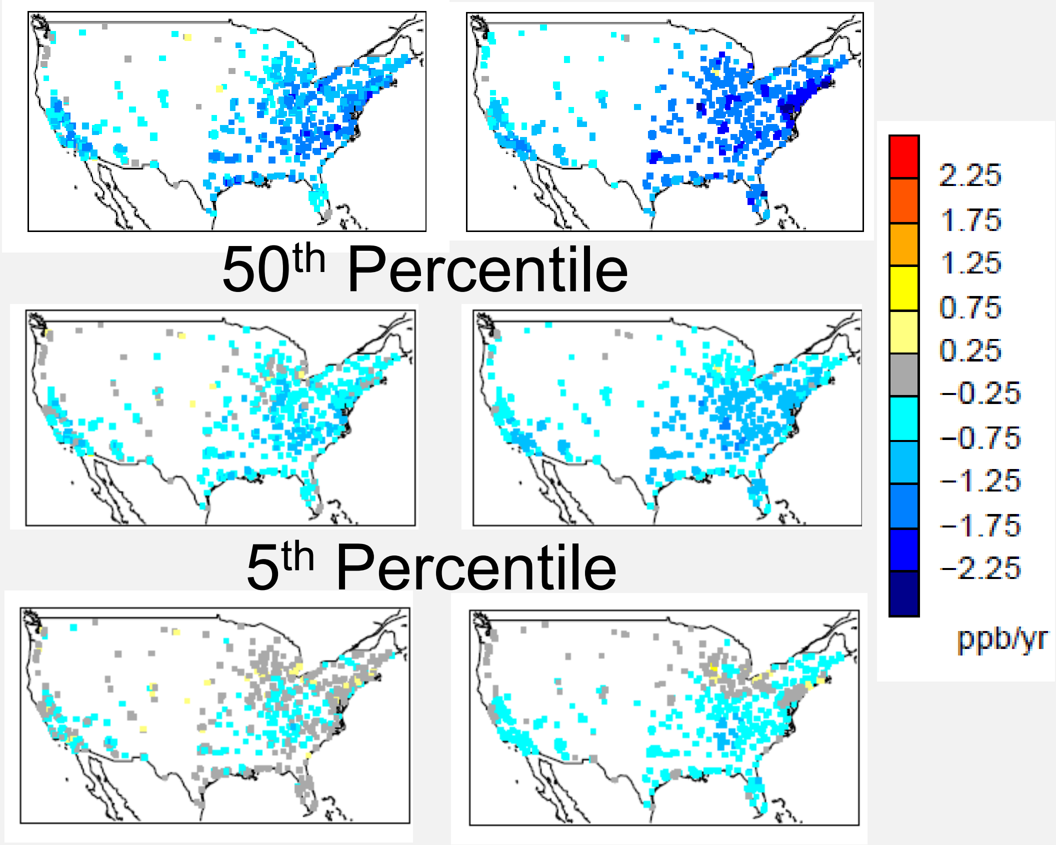
For NO_2, H-CMAQ simulates decreasing trends in North America and Europe and increasing trends in China and India in all seasons

For O_3, summertime trends follow NO_2 trends in all regions while wintertime trends over North America, Europe, and China have the opposite sign of NO_2 trends, indicating the effects of titration

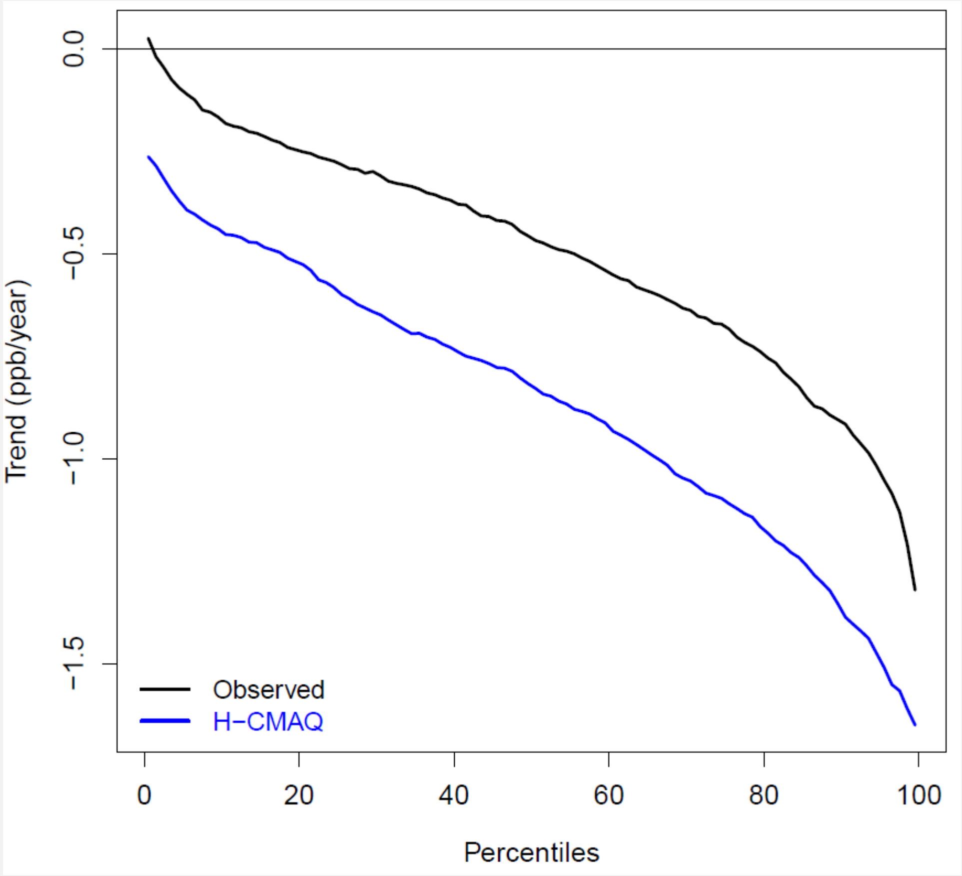
Comparison of Observed and Modeled Trends May-September Surface MDA8 O_3, 2002 – 2017, AQS

Observations H-CMAQ

95th Percentile



Trends by Percentile
Median All Sites



H-CMAQ captures the spatial variation of trends and their variation by percentiles, but overestimates their magnitudes

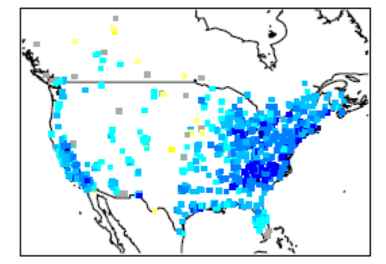
United States Environmental Protection Agency

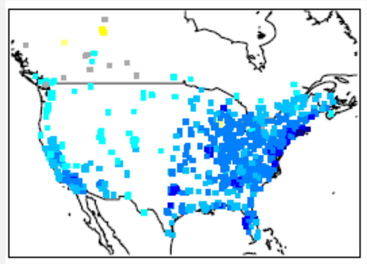
Comparison of Observed and Modeled Trends May-September Surface MDA8 O_3, 2002 – 2014, TOAR

95th Percentile Trends

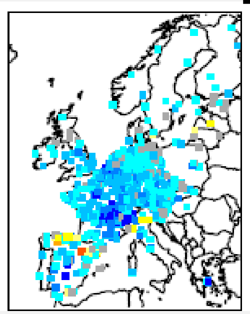
Observations H-CMAQ

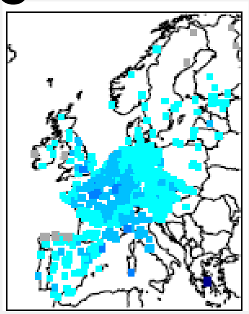
North America



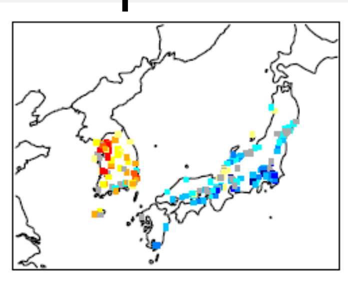


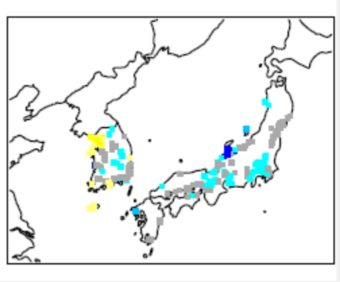
Europe

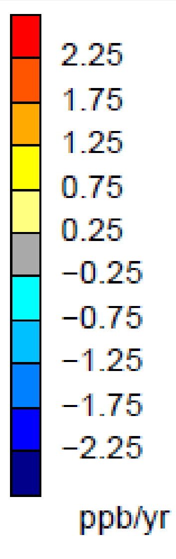




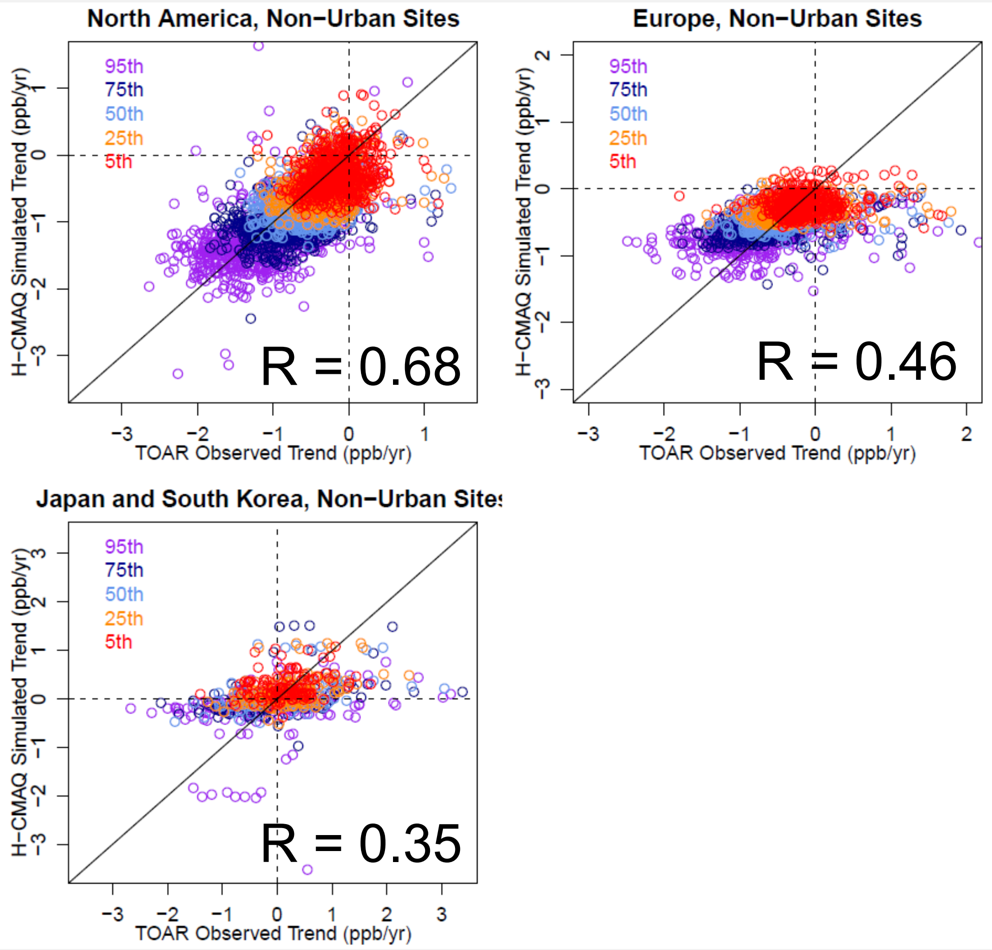
Japan and South Korea







Observed vs. Modeled Trends For Five Percentiles



Except over South Korea, H-CMAQ generally captures the directionality of decreasing 95th percentile trends

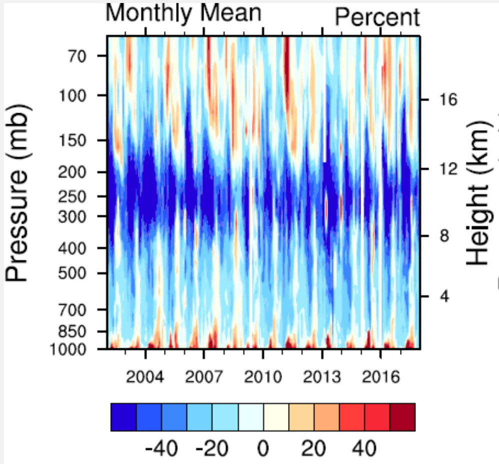
The spatial patterns of trends are captured better for North America than Europe, Japan, and South Korea

Aloft O_3 Performance, Selected Ozonesonde Sites

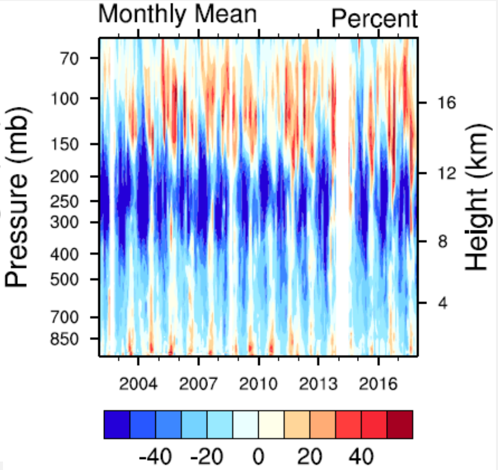
United States Environmental Protection Agency

Time-Height Cross Sections of Percentage Bias in Monthly O_3, 2002 - 2017

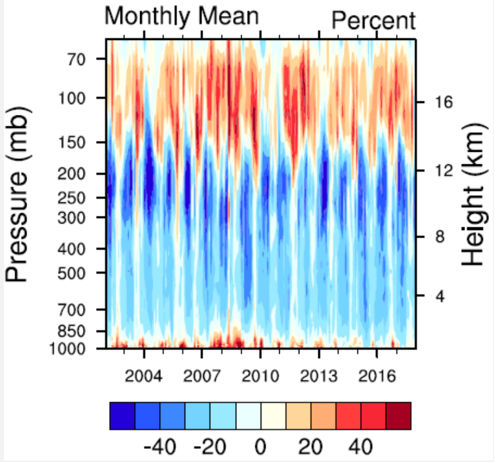
Alert, Canada (82.5° N)



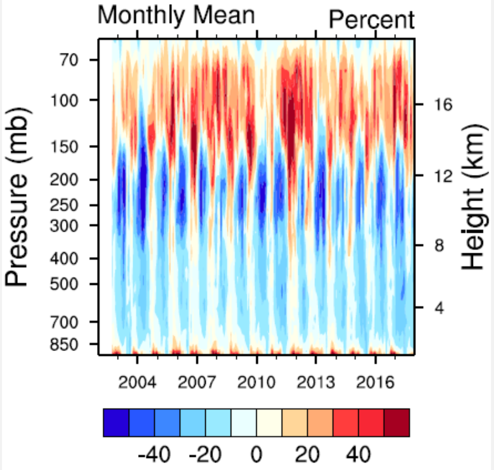
Goose Bay, Canada (53.3° N)



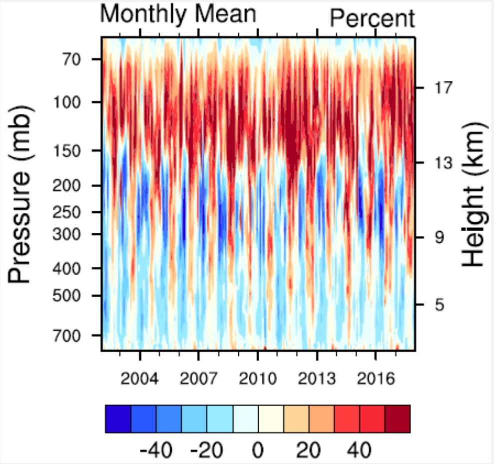
Uccle, Belgium (50.8° N)



Payerne, Switzerland (46.8° N)



Boulder, USA (39.9° N)



Negative upper tropospheric springtime bias, more pronounced for northern stations

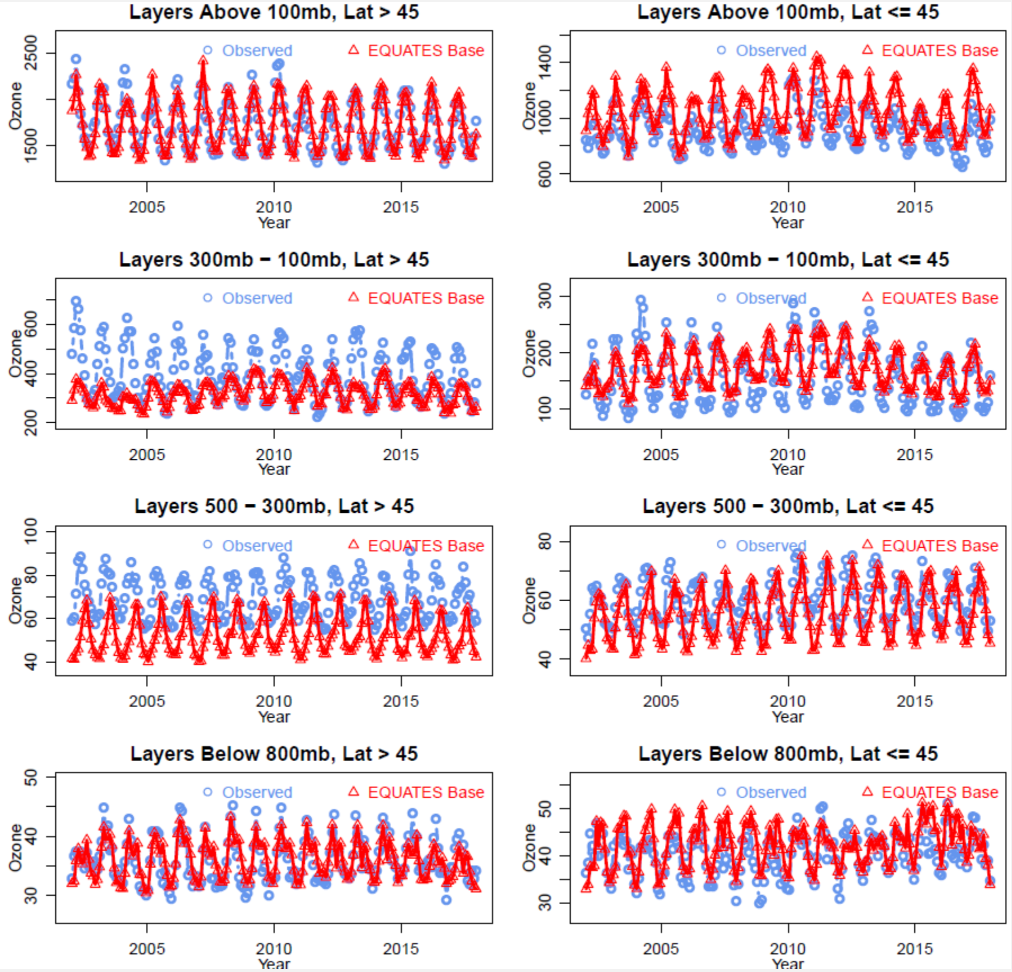
Tendency for positive bias above 150 mb for mid-latitude sites

Aloft O_3 Performance, All Ozonesonde Sites

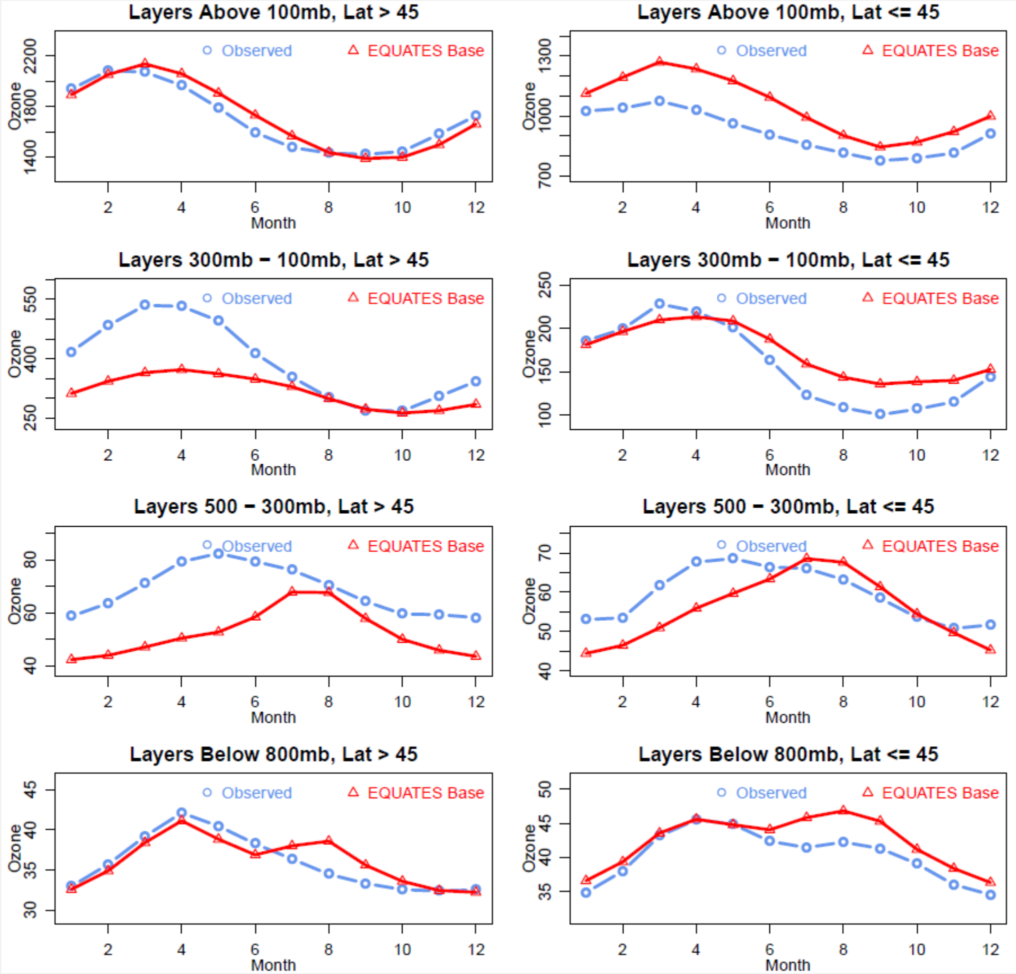
United States Environmental Protection Agency

Monthly Mean O_3, 4 Layer and 2 Latitude Ranges

Monthly Time Series



Average Seasonal Cycle



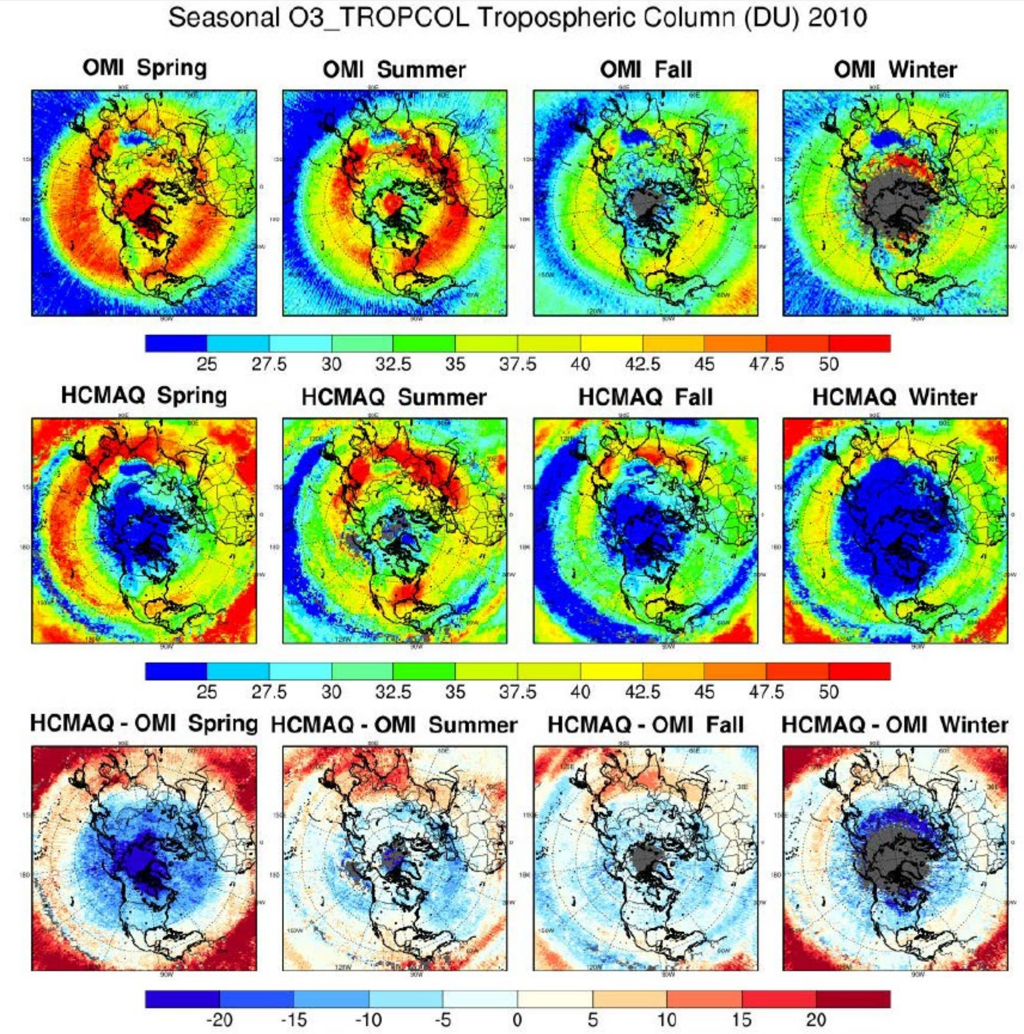
Observations
H-CMAQ

Generally good representation of O_3 above 100 mb

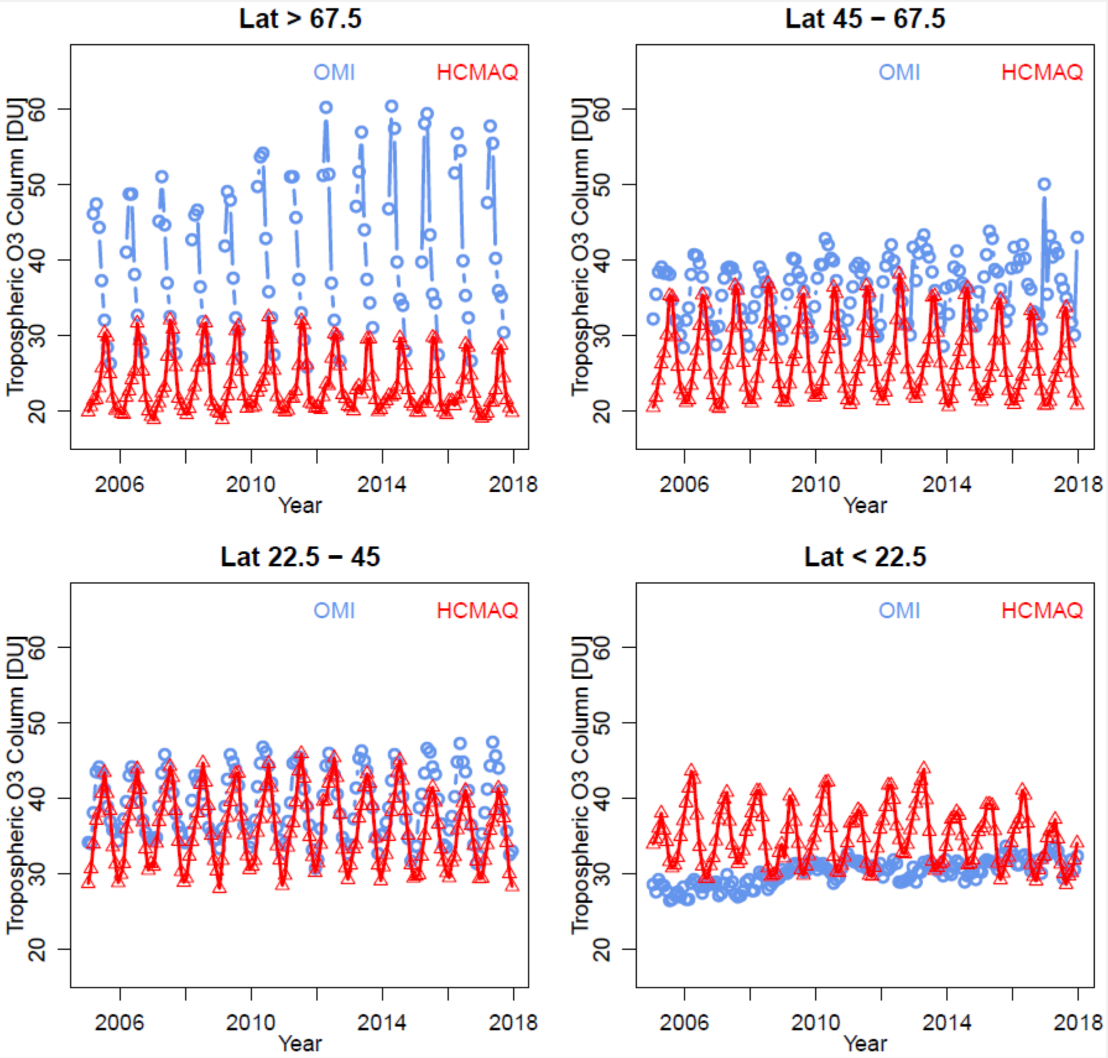
Underestimation of winter and spring O_3 in the mid and upper troposphere, especially at northern latitudes

Satellite Comparisons, Tropospheric Column O_3

Seasonal Columns, example: 2010



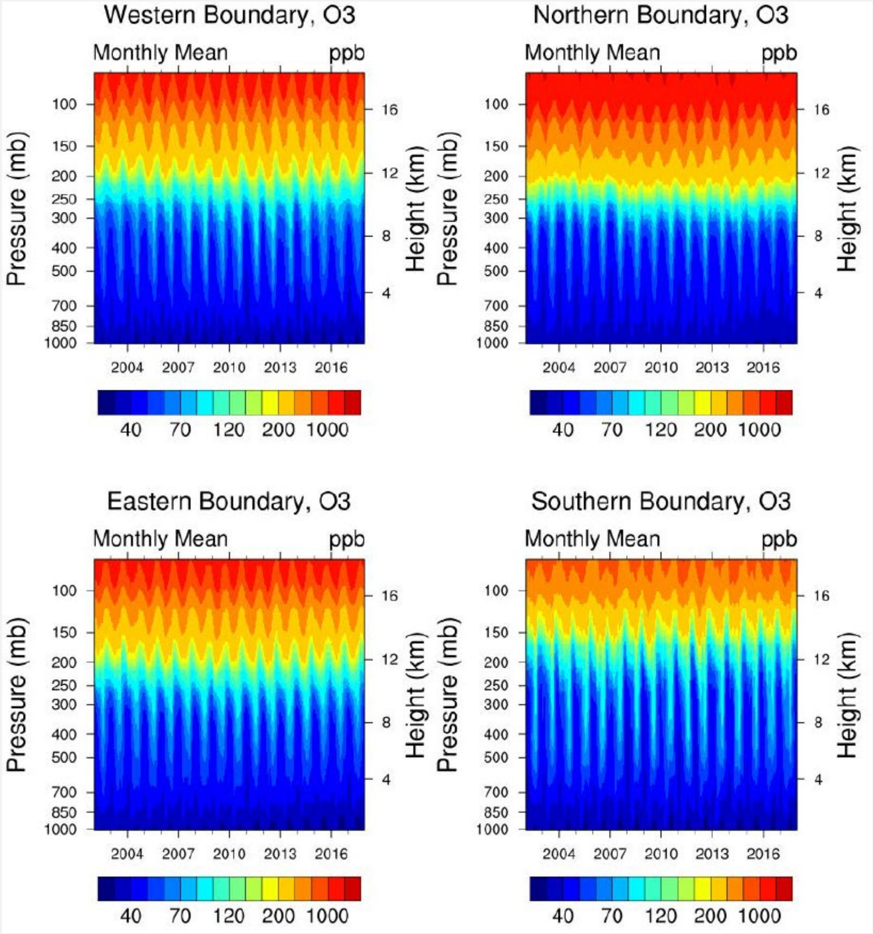
Monthly Time Series

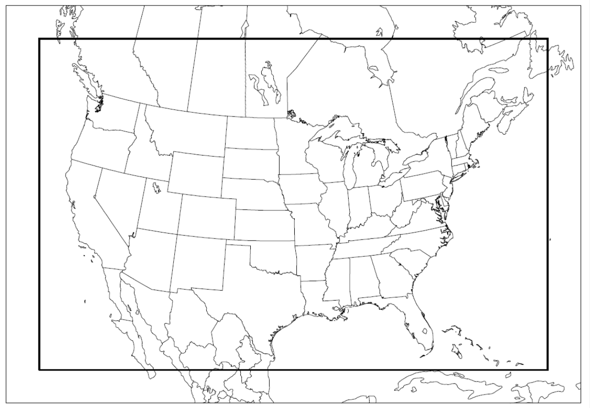


Most pronounced feature, consistent across years: underestimation of tropospheric O_3 column during spring (and to a lesser extent winter) at higher latitudes

O_3 Time Series at Boundaries of 12 km Domain

Monthly Time Series, Cross-Sections

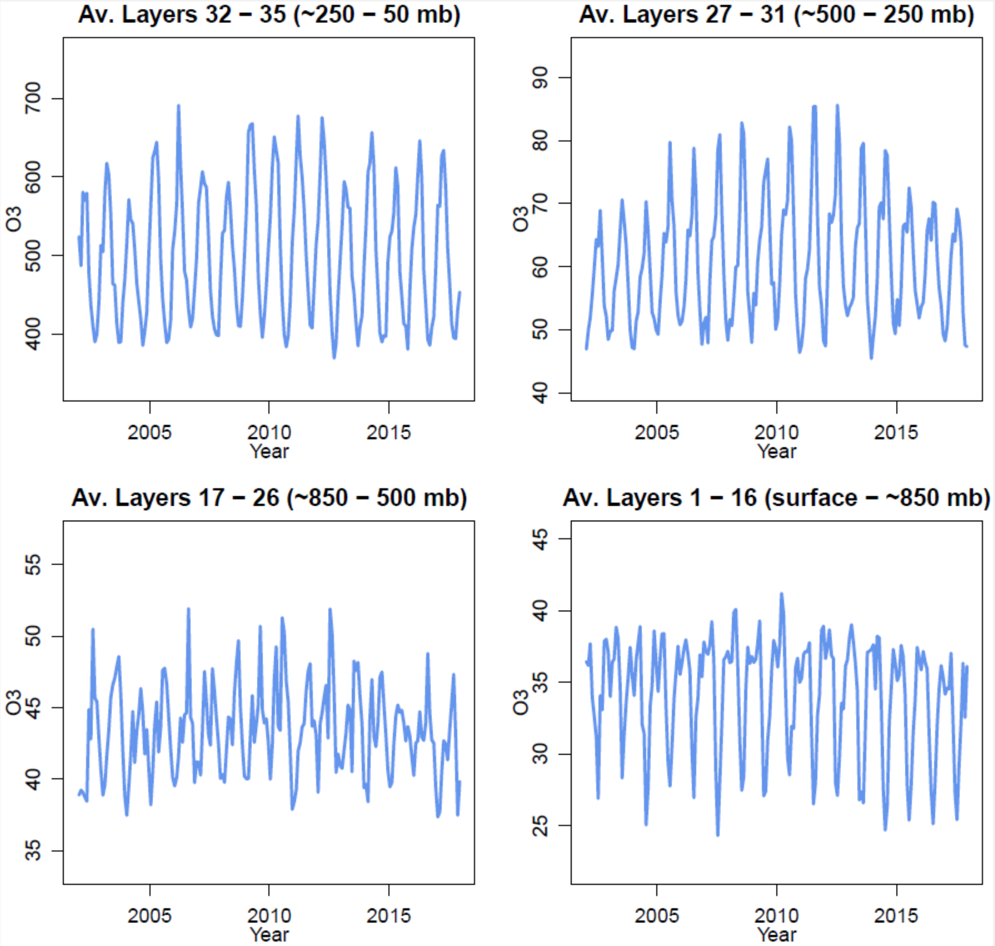




Recent years show downward trends in annual peak values at the western boundary, most pronounced in the free troposphere

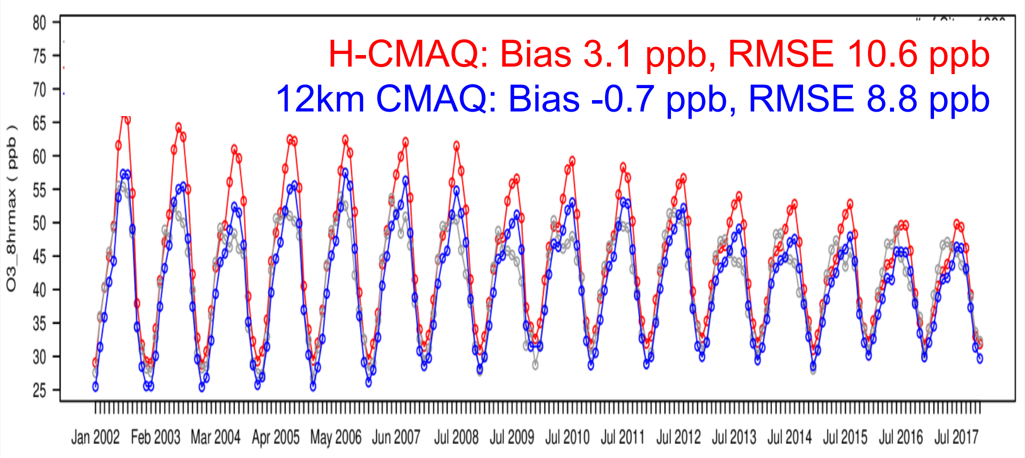
→ See presentation by James East on the effects of satellite assimilation on boundary conditions

Monthly Time Series, Western Boundary

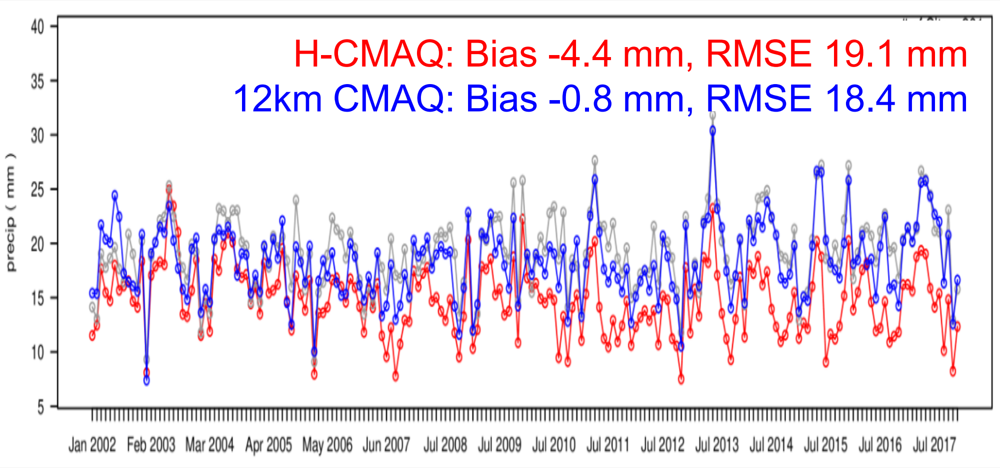


Comparison to 12km CMAQ Simulations: Monthly Mean Time Series

AQS MDA8 O_3

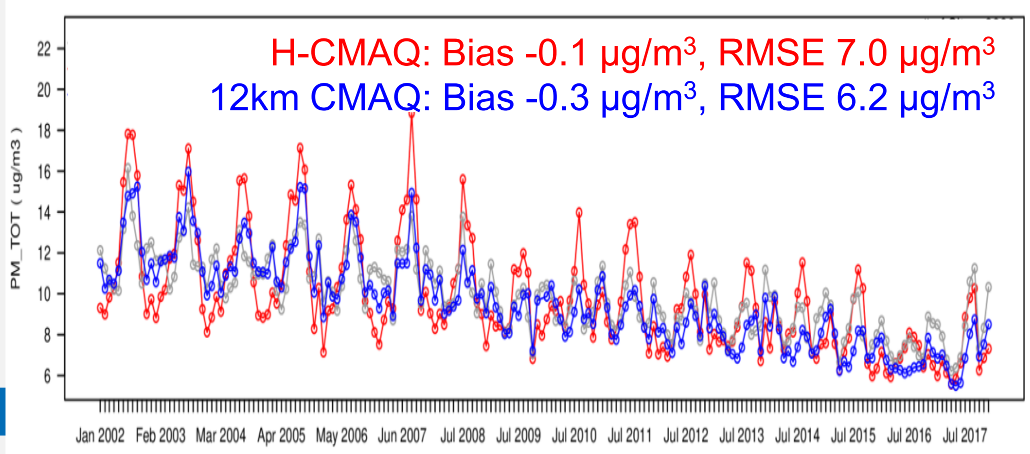


NADP Precipitation



Observations
H-CMAQ
12 km CMAQ

AQS $PM_{2.5}$



Generally better performance for the 12 km CMAQ simulations

H-CMAQ has larger positive summertime MDA8 O_3 and $PM_{2.5}$ biases and larger negative summertime precipitation bias than the corresponding 12 km simulations

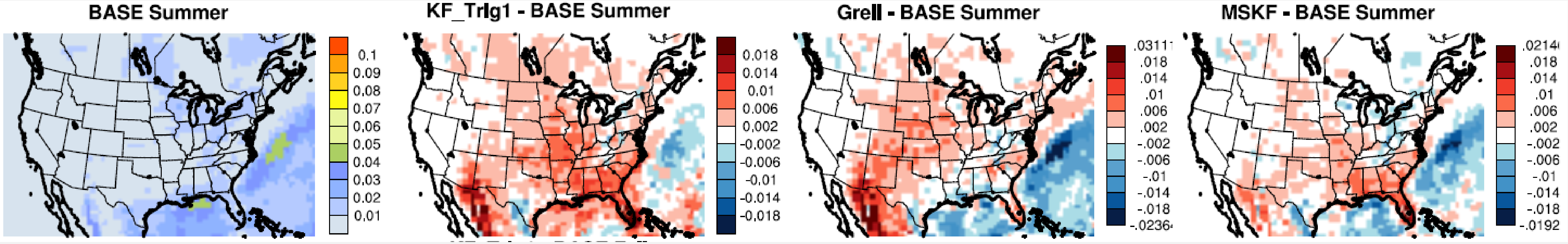
H-CMAQ Sensitivity Simulations

- Key differences to 12 km CMAQ setup:
  - Meteorology - more pronounced summertime dry bias in 108 km than 12 km simulations
  - Biogenic and soil NO emissions (CAMS for H-CMAQ, BEIS for 12 km CMAQ)
- Three sensitivity simulations with alternative WRF cumulus parameterization options:
  - Kain-Fritsch (KF) with trigger 1 instead of trigger 2
  - Grell
  - WRFv4.2.2 with Multi-Scale Kain-Fritsch (MSKF)
- Two sensitivity simulations with alternative options for biogenic emissions:
  - Patch in BEIS from 12 km CMAQ EQUATES simulation to the 108 km grid (no changes for areas of the 108 km grid not covered by the 12 km grid)
  - Test recently developed MEGAN3 inline option, using Yienger-Levy (1995) for soil NO → see presentation by Jeff Willison

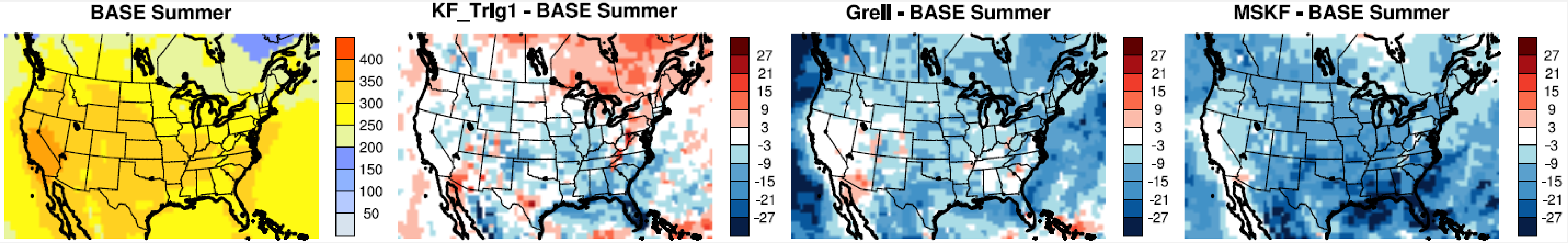
All sensitivity simulations were performed for 2010 only

108 km WRF Cumulus Option Sensitivities – Precipitation and Shortwave Radiation Impacts

Summer Average Precipitation



Summer Average Shortwave Radiation

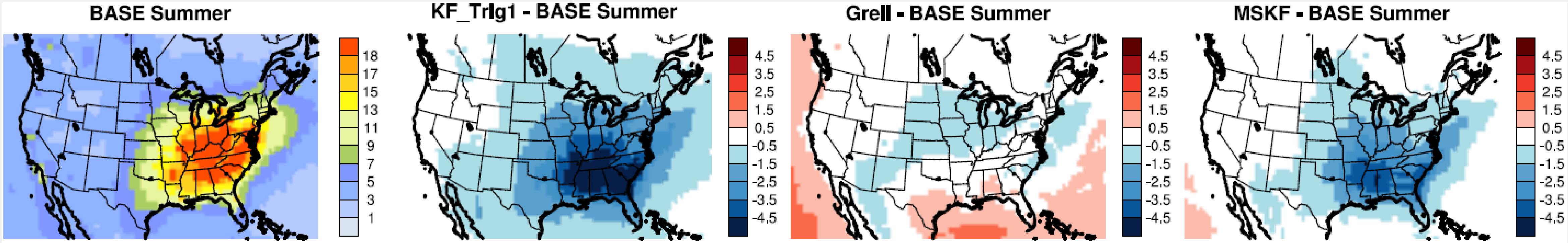


Relative to BASE, all sensitivities tend to simulate higher summertime precipitation and correspondingly lower shortwave radiation

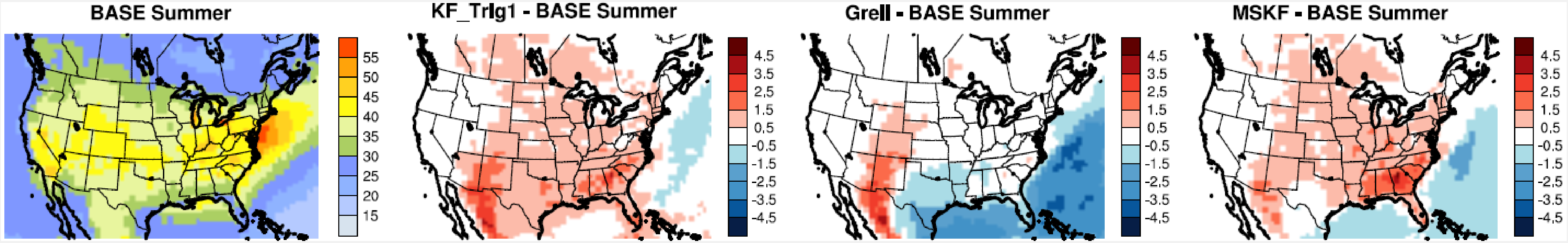
United States Environmental Protection Agency

108 km WRF Cumulus Option Sensitivities – $PM_{2.5}$ and O_3 Impacts

Summer Average $PM_{2.5}$



Summer Average O_3



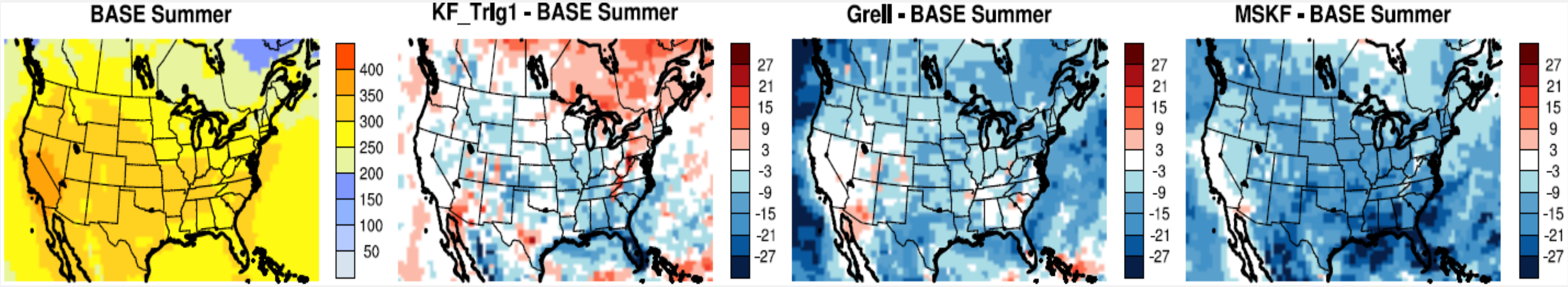
Convective schemes have a pronounced impact on warm season $PM_{2.5}$ concentrations

The impact on O_3 is less pronounced and has the opposite sign of the $PM_{2.5}$ impact

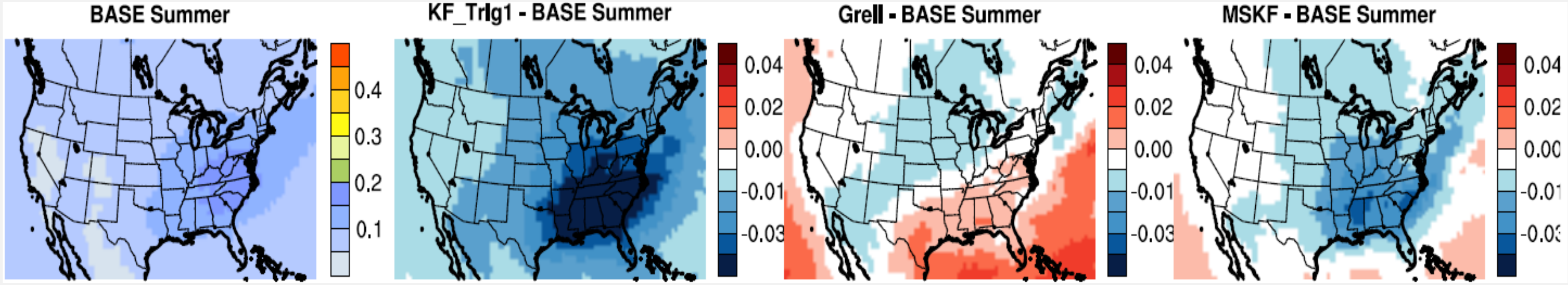
United States Environmental Protection Agency

108 km WRF Cumulus Option Sensitivities – Shortwave Radiation, AOD, and Photolysis Rates

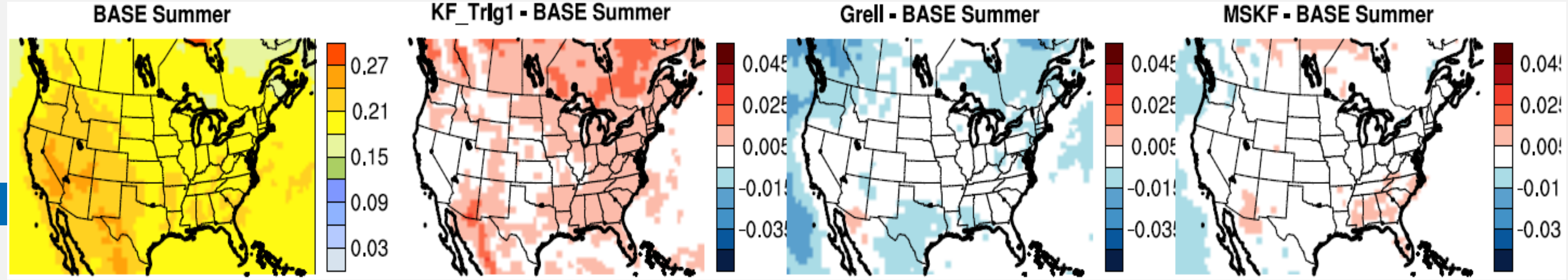
Summer Average Shortwave Radiation



Summer Average AOD



Summer Average JNO2



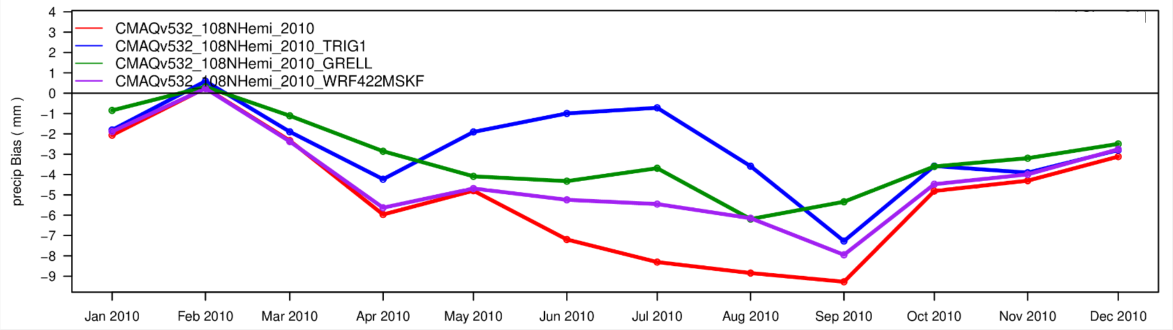
Increased precipitation and consequently lower $PM_{2.5}$ relative to BASE reduces AOD for KF trigger 1 and MSKF

This counteracts the effects of decreased shortwave radiation, leading to enhanced photolysis and resulting in higher O_3 over regions of increased precipitation and decreased $PM_{2.5}$

EPA
United States
Environmental Protection
Agency

Impact on H-CMAQ Biases

Precipitation, NADP



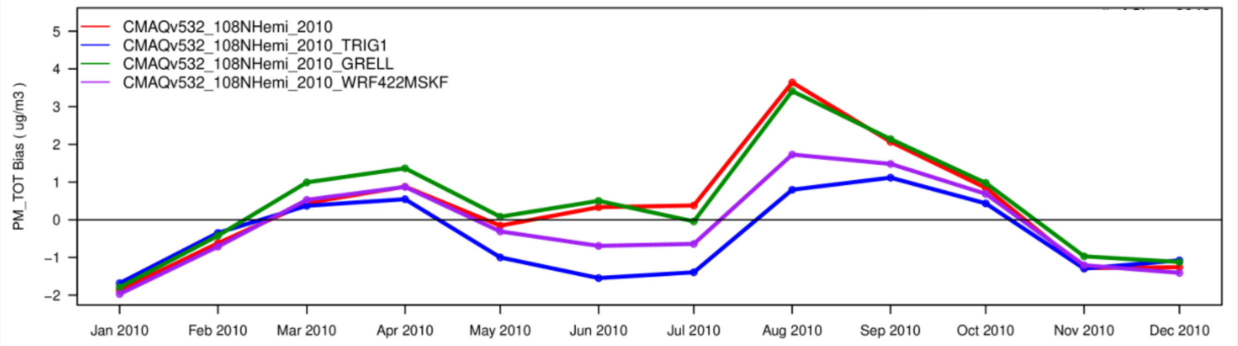
BASE

KF Trigger 1

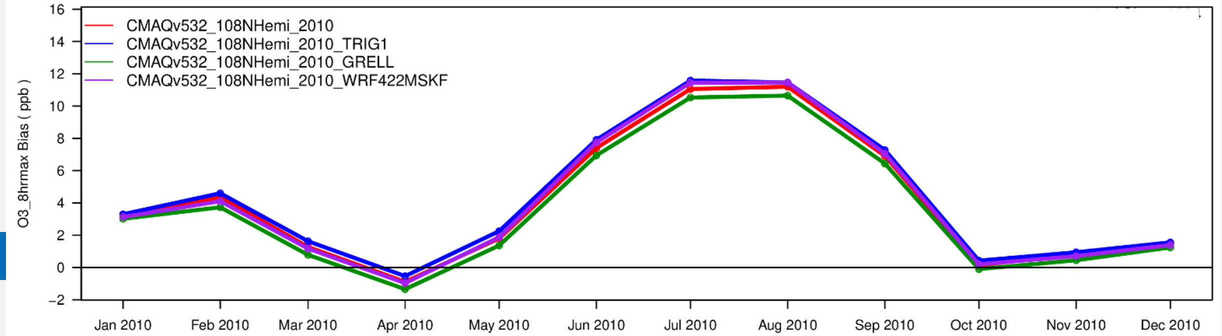
Grell

MSKF

$PM_{2.5}$, AQS



MDA8 O_3, AQS



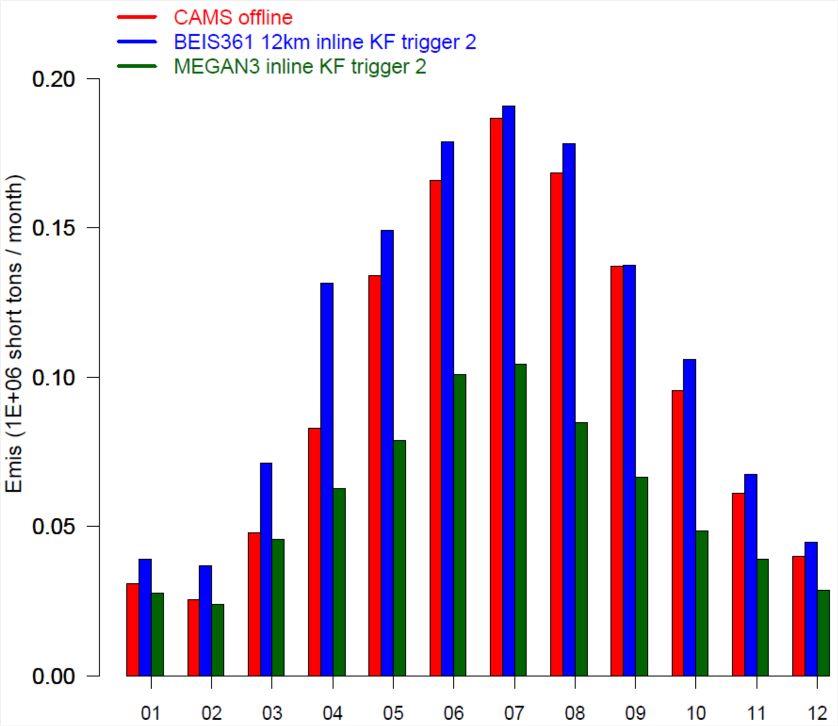
Convective schemes have a pronounced impact on warm season precipitation and $PM_{2.5}$ bias

KF trigger 1 shows the largest improvement in summertime dry bias, but slightly increases MDA8 O_3 bias due to increased photolysis resulting from lower AOD

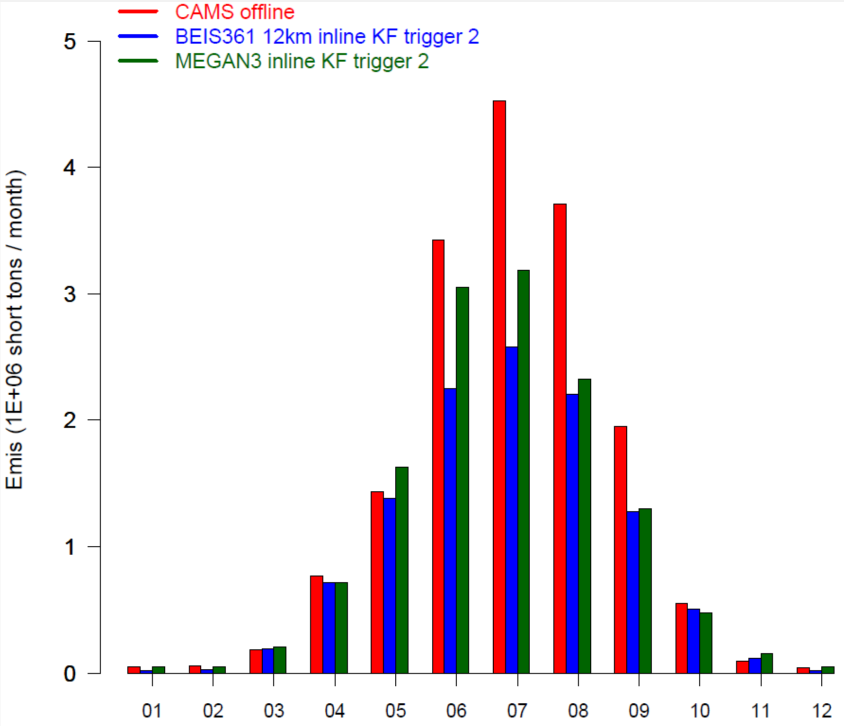
108 km Biogenic Emission Sensitivities

108 km Biogenic Emissions over the U.S.

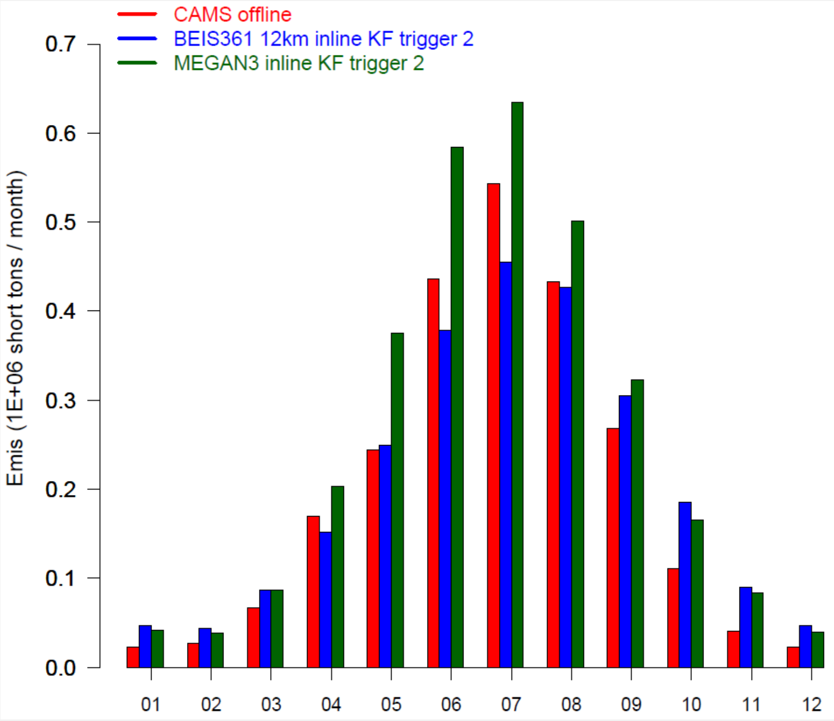
Soil NO



Biogenic Isoprene



Biogenic Monoterpenes



BASE – CAMS offline
BEIS from 12 km simulation
MEGAN3 inline

MEGAN3 inline soil NO lower than CAMS and BEIS

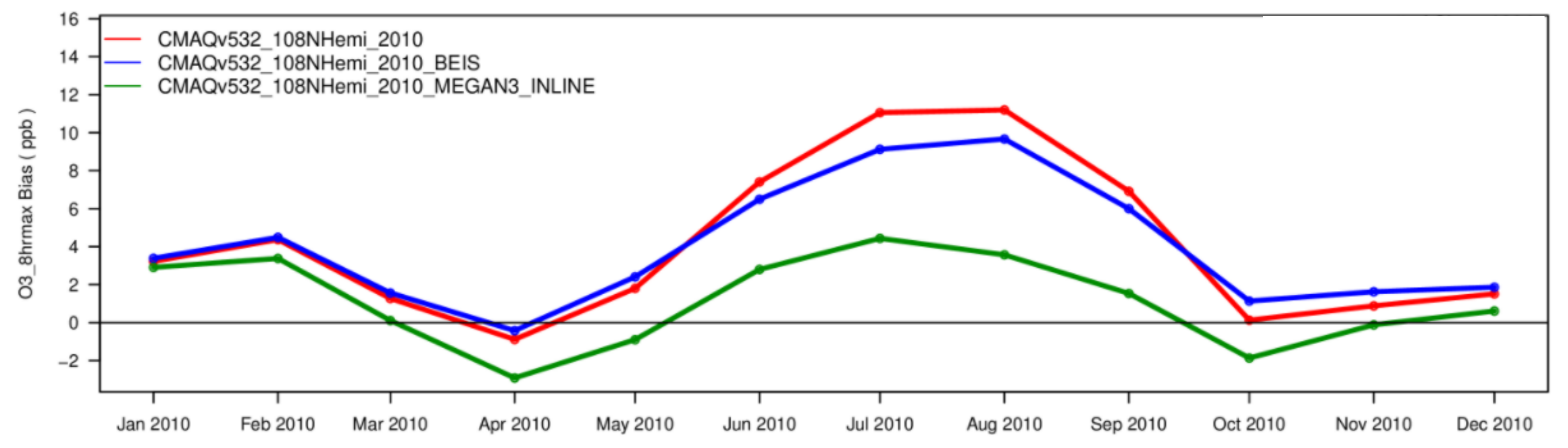
BEIS and MEGAN3 inline isoprene lower than CAMS

MEGAN3 monoterpenes higher than CAMS and BEIS

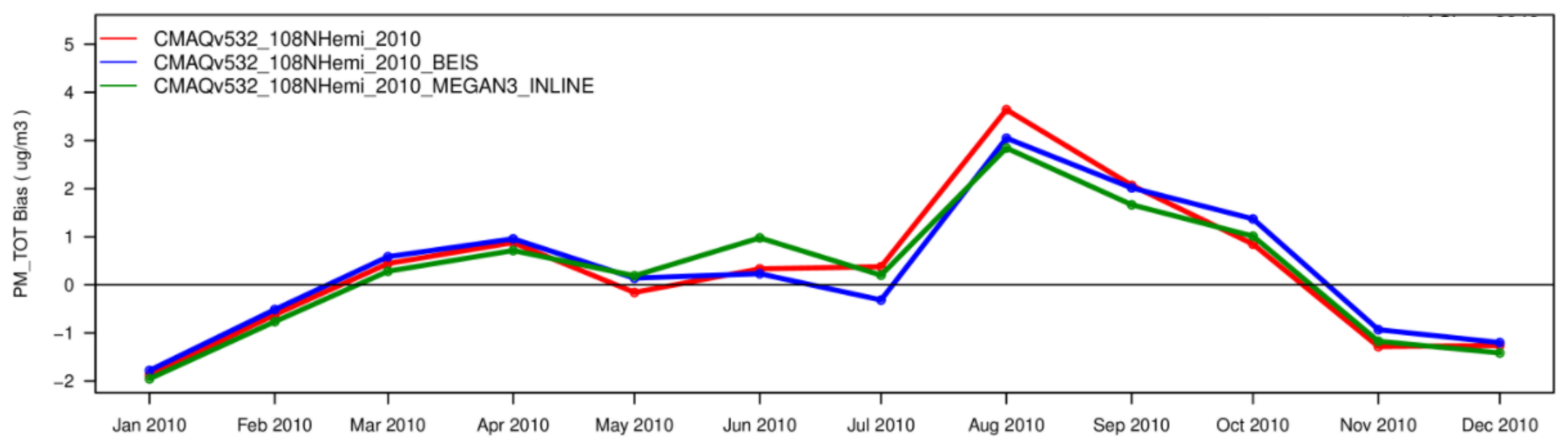
United States Environmental Protection Agency

Impact on H-CMAQ Biases

MDA O_3, AQS



$PM_{2.5}$, AQS



BASE (CAMS offline)
BEIS from 12 km simulation
MEGAN3 inline

For O_3, lowest summertime biases with MEGAN3 (lower soil NO)

$PM_{2.5}$ sensitivity to biogenic emissions is smaller than the sensitivity to cumulus parameterization shown earlier

United States Environmental Protection Agency

Summary

- EQUATES 2002 – 2017 108 km H-CMAQ simulations:
  - Persistent summertime surface O_3 overpredictions and tendency to underestimate springtime O_3 at the surface as well as aloft
  - H-CMAQ captures the spatial variation of O_3 trends and their dependence on percentiles, but tends to overestimates their magnitude
  - Recent years show downward trends in O_3 inflow at the western boundary of the 12 km CMAQ domain
- Additional 108 km H-CMAQ sensitivity simulations for 2010 show:
  - Pronounced impact of WRF cumulus options on precipitation and $PM_{2.5}$ with competing effects for O_3
  - Strong O_3 sensitivity to MEGAN3 inline emissions, likely due to lower soil NO
- Daily average 3D H-CMAQ output fields will be made available to the community via the CMAS data warehouse

Also see the presentations by **Jeff Willison**, **Mike Madden**, and **James East** and posters by **Rebecca Miller** and **Daiwen Kang** for related work